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13. ABSTRACT (Maximum 200 Words)

This report summarizes the work performed by Spectral Sciences Inc. (SSI) during FY under the SERDP program for atmospheric radiance algorithm optimization. The task consisted of (1) adding infrared CFC cross sections and concentration profiles to MODTRAN for transmittance and radiance calculations, and (2) investigation the use of MODTRAN for radiative flux calculations, as a step towards assessing the effects of flux alterations brought about by anthropogenic changes in trace constituents.

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OPTIMIZATION OF ATMOSPHERIC RADIANCE ALGORITHMS FOR REMOTE SENSING:

MODTRAN UPGRADES AND APPLICATIONS

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1. INTRODUCTION

This report summarizes the work performed by Spectral Sciences Inc. (SSI) during FY93 under the SERDP program for atmospheric radiance algorithm optimization. The tasks consisted of (1) adding infrared CFC cross sections and concentration profiles to MODTRAN for transmittance and radiance calculations, and (2) investigating the use of MODTRAN for radiative flux calculations, as a step towards assessing the effects of flux alterations brought about by anthropogenic changes in trace constituents.

2. INCORPORATION OF CFC'S INTO MODTRAN

The objective of this task was to upgrade the MODTRAN code[1,2] to include chlorofluorocarbons (CFCs), which can be significant atmospheric absorbers or emitters in the lower atmosphere. The CFCs included are those for which cross section data are available in HITRAN-92;[3,4] these are CFC-11 (CCl_3F), CFC-12 (CCl_2F_2), CFC-13 ($CClF_3$), CFC-14 (CF_4), CFC-22 (CHF_2Cl), CFC-113 ($C_2Cl_3F_3$), CFC-114 ($C_2Cl_2F_4$) and CFC-115 (C_2ClF_5). These species are currently supported in FASCODE;[5] MODTRAN achieves as close agreement as possible with FASCODE within the available resolution. This project was carried out with the assistance of J. Chetwynd (PL) and in consultation with G. Anderson (PL).

The HITRAN-92 database contains high-resolution, temperature-dependent cross sections σ, in units of cm^2/molecule, that are used in the transmittance expression $\exp(-\sigma\eta)$, where η is the line-of-sight absorber density. For example, CFC-11 has cross-sections listed from 830.0010 cm^{-1} to 859.9960 cm^{-1} for 5 different temperatures. There are 2023 entries for each temperature; thus each entry corresponds to a spectral bin of (859.9960-830.0010)/2023 cm^{-1} or 0.01302 cm^{-1}. CFC-11 also has cross-section values listed from 1060.0090 to 1106.9890 cm^{-1}.

For use in MODTRAN, the HITRAN-92 cross sections were binned into 1 cm^{-1} bins using a trapezoidal algorithm and integrated into MODTRAN's transmittance and radiance routines. It was decided to upgrade the code only in the MODTRAN mode (as opposed to the LOWTRAN mode). Altitude profiles for the default CFC number densities have been taken from FASCODE. In addition, the capability for implementing user-defined CFC profiles has been implemented; the method is analogous to inputing species profiles using TAPE5 for MODEL 0 or 7.

The new MODTRAN coding is quite general. It can handle any number of new species as set by a PARAMETER statement. If the user wishes to perform calculations on species other than CFCs, only two files need modification. The first is a block data file which contains species profiles, names and atomic weights. The second file that needs to be modified contains the cross sections. The general nature of the coding has two

benefits: (1) additional species can be incorporated, and (2) code validation is facilitated by testing it on species whose transmittances and radiances are already known.

The accuracy of the new version of MODTRAN has been validated by comparing results with FASCODE calculations. An illustrative comparison of CFC band radiances appears in Figure 1. While there are small differences between the codes in the neighboring CO_2 and O_3 band regions, the agreement is virtually exact for the CFC bands.
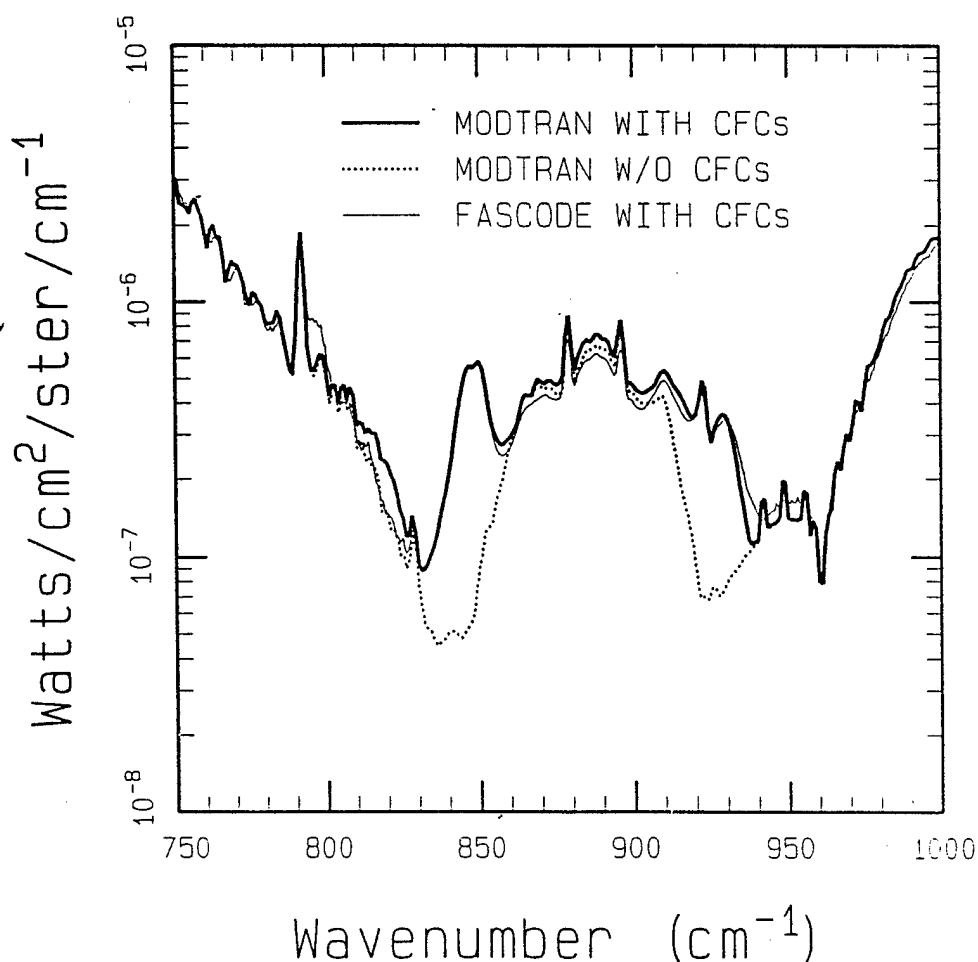

Figure 1. Comparison of MODTRAN and FASCODE Calculations Showing CFC Emission Spectra for 12 km Limb View, 1976 US Standard Atmosphere.

3. RADIATIVE FLUX CALCULATIONS USING MODTRAN

The objective of this effort was to perform a preliminary investigation of the usefulness of MODTRAN for atmospheric radiative flux calculations. This work was carried out in collaboration with and under the supervision of G. Anderson (Phillips Laboratory) and co-workers.

Using a research version of MODTRAN, radiative cooling calculations were carried out for several cases for which FASCODE results are available. A MODTRAN-FASCODE comparison is shown in Figures 2 and 3. These calculations are for H_2O only and include both the molecular line and continuum components. The agreement is very promising.

The small differences between the MODTRAN and FASCODE radiative cooling results are due to several factors, including differences in the number and selection of the atmospheric layers and inherent differences between the line-by-line and band model approaches. In particular, we have identified a source of inaccuracy in MODTRAN emissivity calculations associated with temperature gradients within opaque atmospheric layers. In "exact" frequency-grid codes, temperature gradients are typically handled using the "linear-in-tau" approach, which assumes that changes in optical depth and temperature are proportional throughout the layer. There is no equivalent approach in band model-based codes, in which the optical depth is a spectral interval-averaged quantity.

In a follow-on effort, we are addressing this layer temperature gradient problem in MODTRAN using a new, computationally efficient, accurate, and general method based on a Padé expansion of the curve of growth.[6] Further investigations, including comparisons to the ICRCCM (InterComparison of Radiation Codes in Climate Models) data base, are also being pursued and will enable a more complete evaluation of the applicability of MODTRAN to radiative flux problems.[7]

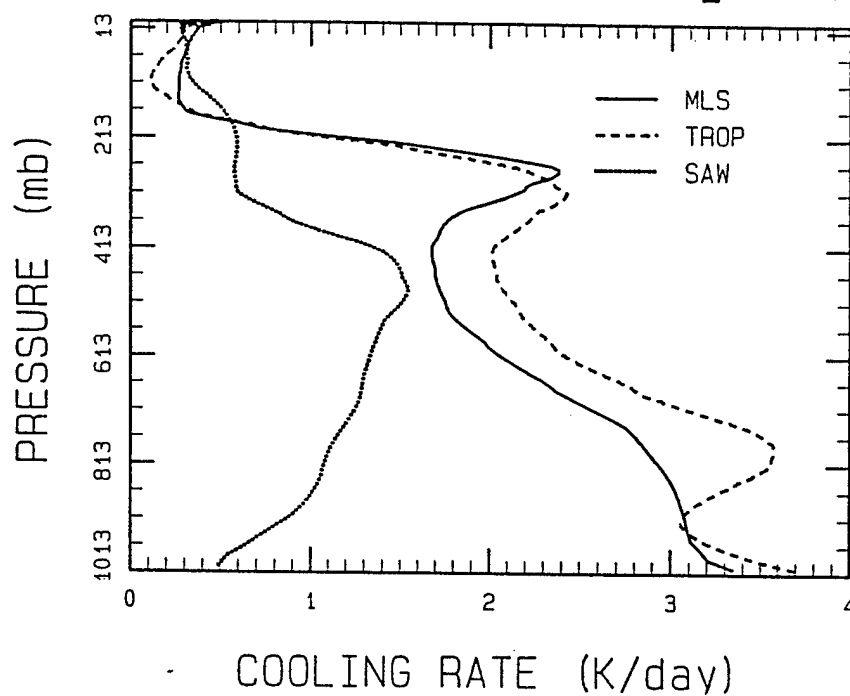## 10-3,000 cm^{-1} ICRCCM Profiles H$_2$O Only

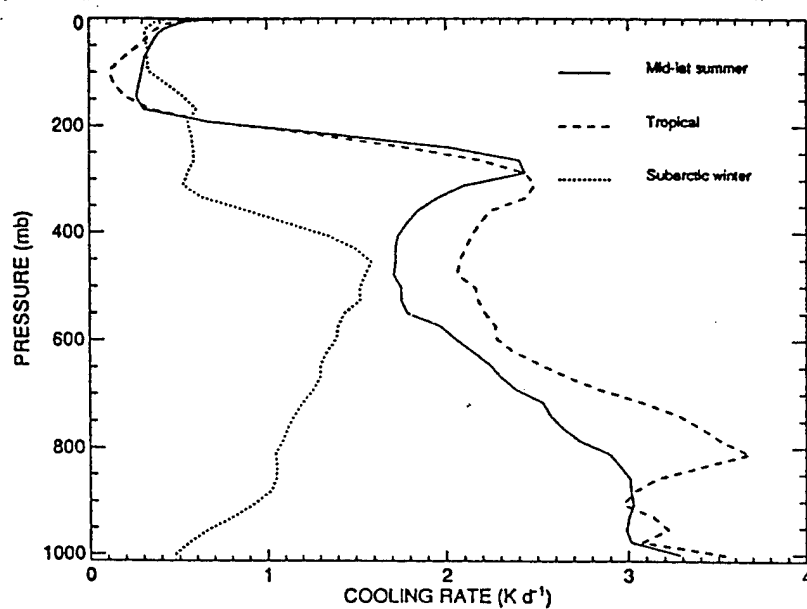Figure 2. MODTRAN Radiative Flux Calculations for Different Model Atmospheres.

Figure 3. FASCODE Radiative Flux Calculations for the Model Atmospheres of Figure 2.

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